APPENDIX A

Models-3 Directory Tree

The Models-3 tree is usually housed in D:\models3. This may be configured to be a different directory during installation. The name must not contain any capital letters. This top-level directory is identified by the environment variable %M3HOME%. The five main sections of the tree are:

- *datasets* - %M3DATA%: Inputs and outputs to studies reside in .\studies and .\nostudies. This will be the area that is prone to the most growth as far as disk space is concerned.

- *exec* - %M3HOME%\exec: Executables that have been tagged as "official" are placed in this area. The users have permissions to modify this area. There will be subdirectories for models and each hardware platform.

- *framework* - %M3HOME%\framework: Programs that allow the users to run the suite of tools and models are stored in this directory along with the database and Orbix configuration files. Users have privileges to modify the database files only.

- *models* - %M3HOME\models: Scientific models are stored in this area. The conforming models are written in FORTRAN and must be compiled before they are run. The users in group "models3" have permissions to modify this area.

- *tools* - %M3HOME%\tools: Third-party tools, freeware, and scripts that kick off commercial executables from the framework. The users do not have permissions to change the contents of this directory.

The top two levels of the tree are as follows:

```
datasets:
nostudies\          studies\

exec:
protected\

framework:
bin\      config\    db\       installdb\  lib\      templates\

models:
CCTM\   ICON\   MCIP\   LUPROC\   MECH\  include\
ECIP\    BCON\   JPROC\ PROCAN\  PDM\ SMOKETOOL\
```

tools:
GridViewer\ Models3Vis\ VisDriver\ M3SubsetTool\ mm5_to_v5d\
IOAPI\ PAVE\ arc\ netCDF\ sas\ STENEX\ stenex\
MP\ Vis5d\ build\ rcs_cvs\ M3GridSample\ to_v5d\ smoke\

The complete listing of all files that were used to create the framework and models code are in %M3HOME%\framework\installdb\BillOfMaterials.txt. It also contains a listing of every file included on the latest installation tape.

APPENDIX B

Models-3 Environment Variables

The following environment variables are used by the Models-3 system. They are set in the m3env.bat script.

Environment Variable	Value	Description
Models-3 Directories		
M3HOME	usually D:\models3	base directory where software is installed
M3FRAME	%M3HOME%\framework	framework files and database
	%M3HOME%\datasets	datasets
M3EXEC	%M3HOME%\exec	executables - compiled models
M3TOOLS	%M3HOME%\tools	tools to use - do not compile these
M3MODEL	%M3HOME%\models	source code for scientific models
M3FBIN	%M3FRAME%\bin	framework binary executables
M3FLIB	%M3FRAME%\lib	framework libraries
M3FSRC	%M3FRAME%\src	framework source - empty for most sites
M3FINC	%M3FRAME%\inc	framework include files - empty for most sites
M3FDBPATH	%M3FRAME%\db	framework database files
M3FDBNAME	%M3FDBPATH%\models3.db	main framework database
M3MCTM	%M3MODEL%\CCTM	CTM model (chemistry)
M3MSTOOL	%M3MODEL%\smoketool	Smoke Tool source code and libraries
M3TEMP	usually it is /tmp or C:\TEMP	holds temporary files
Other		
M3SITE	(system dependent)	unique site name
M3HOST	(system dependent)	host name, including domain name
M3FMHOST	(system dependent)	host name where File Migrator is running
M3USERHOME	(system dependent)	the user's home directory

Table B-1. Models-3 Framework Environment Variables

APPENDIX C

Selected Dataset Details

The following table describes selected datasets under the nostudies area. Acronyms may be found in Appendix B of User Manual.

Key: M is Main. Main datasets are distributed with the Models-3 Software.
S is Supplemental. Supplemental datasets are available separately from EPA and/or NTIS.

TABLE C-1. Selected Datasets Under Nostudies

Dataset Name	File Location	Tape
BC profile data for BCON	%M3DATA%\nostudies\bcon\bc_profile_v5.dat	M
IC profile data for ICON	%M3DATA%\nostudies\bcon\ic_profile_v5.dat	M
Land-use data for LUPROC	%M3DATA%\nostudies\bcon\mm5_soil_data	M
Hourly ozone measurements July 6-10, 1995 (SAS)	%M3DATA%\nostudies\ozone\o3_dev.ssd01	M
Hourly ozone measurements July 11-15, 1995 (SAS)	%M3DATA%\nostudies\ozone\o3_evl.ssd01	M
Site locations for all available monitoring stations for July 6-15, 1995 (SAS)	%M3DATA%\nostudies\ozone\site.ssd01	M
Hourly ozone measurements from NARSTO for 1995	%M3DATA%\nostudies\narsto_ne_1995\ AME07AI1.1HR	M
Description of NARSTO Data	%M3DATA%\nostudies\narsto_ne_1995\ narsto_ne_readme95.txt	M
Extra-terrestrial irradiance values for JPROC	%M3DATA%\nostudies\phot\ETirradiance.dat	M
Vertical Profiles data for JPROC	%M3DATA%\nostudies\phot\PROFILES.dat	M

TABLE C-1. Selected Datasets Under Nostudies		
Dataset Name	File Location	Tape
O2 absorption cross section data for JPROC	%M3DATA%\nostudies\phot\O2_NASA94	M
O2 absorption cross section data for JPROC	%M3DATA%\nostudies\phot\O2_RADM88	M
O3 Photolysis to O1D for JPROC	%M3DATA%\nostudies\phot\O3O1D_NASA94	M
O3 Photolysis to O1D for JPROC	%M3DATA%\nostudies\phot\O3O1D_RADM88	M
O3 Photolysis to O1D for JPROC	%M3DATA%\nostudies\phot\O3O1D_CBIV88	M
O3 Photolysis to O3P for JPROC	%M3DATA%\nostudies\phot\O3O3P_RADM88	M
O3 Photolysis to O3P for JPROC	%M3DATA%\nostudies\phot\O3O3P_NASA94	M
Nitrogen Dioxide Photolysis for JPROC	%M3DATA%\nostudies\phot\NO2_RADM88	M
Nitrogen Dioxide Photolysis for JPROC	%M3DATA%\nostudies\phot\NO2_CBIV88	M
Nitrogen Dioxide Photolysis for JPROC	%M3DATA%\nostudies\phot\NO2_NASA94	M
Nitrate Photolysis to NO for JPROC	%M3DATA%\nostudies\phot\NO3NO_RADM88	M
Nitrate Photolysis to NO for JPROC	%M3DATA%\nostudies\phot\NO3NO_NASA-94	M
Nitrate Photolysis to NO2 for JPROC	%M3DATA%\nostudies\phot\ NO3NO2_RADM88	M
Nitrate Photolysis to NO2 for JPROC	%M3DATA%\nostudies\phot\ NO3NO2_NASA94	M
Nitrous Acid Photolysis for JPROC	%M3DATA%\nostudies\phot\HONO_RADM88	M

TABLE C-1. Selected Datasets Under Nostudies		
Dataset Name	File Location	Tape
Nitrous Acid Photolysis for JPROC	%M3DATA%\nostudies\phot\HONO_NASA94	M
Nitric Acid Photolysis for JPROC	%M3DATA%\nostudies\phot\ HNO3_RADM88	M
Nitric Acid Photolysis for JPROC	%M3DATA%\nostudies\phot\ HNO3_NASA94	M
Pernitric Acid Photolysis for JPROC	%M3DATA%\nostudies\phot\HNO4_RADM88	M
Pernitric Acid Photolysis for JPROC	%M3DATA%\nostudies\phot\HNO4_NASA94	M
Hydrogen Peroxide Photolysis for JPROC	%M3DATA%\nostudies\phot\H2O2_RADM88	M
Hydrogen Peroxide Photolysis for JPROC	%M3DATA%\nostudies\phot\H2O2_NASA94	M
Formaldehyde Photolysis to Radicals for JPROC	%M3DATA%\nostudies\phot\ HCHOrad_RADM88	M
Formaldehyde Photolysis to Radicals for JPROC	%M3DATA%\nostudies\phot\HCHOrad_CBIV 88	M
Formaldehyde Photolysis to Radicals for JPROC	%M3DATA%\nostudies\phot\ HCHOrad_NASA94	M
Formaldehyde Photolysis to Molecular Hydrogen for JPROC	%M3DATA%\nostudies\phot\ HCHOmol_RADM88	M
Formaldehyde Photolysis to Molecular Hydrogen for JPROC	%M3DATA%\nostudies\phot\ HCHOmol_CBIV88	M
Formaldehyde Photolysis to Molecular Hydrogen for JPROC	%M3DATA%\nostudies\phot\ HCHOmol_NASA94	M
Acetaldehyde Photolysis for JPROC	%M3DATA%\nostudies\phot\ALD_RADM88	M

TABLE C-1. Selected Datasets Under Nostudies		
Dataset Name	File Location	Tape
Acetaldehyde Photolysis for JPROC	%M3DATA%\nostudies\phot\ALD_CBIV88	M
Acetone Photolysis for JPROC	%M3DATA%\nostudies\phot\ ACETONE_RADM88	M
Methyl Ethyl Ketone Photolysis for JPROC	%M3DATA%\nostudies\phot\ KETONE_RADM88	M
Glyoxal Photolysis to Formaldehyde for JPROC	%M3DATA%\nostudies\phot\ GLYform_RADM88	M
Methyl Glyoxal Photolysis for JPROC	%M3DATA%\nostudies\phot\MGLY_RADM88	M
Unsaturated Dicarbonyl Photolysis for JPROC	%M3DATA%\nostudies\phot\UDC_RADM88	M
Methyl Hydrogen Peroxide Photolysis for JPROC	%M3DATA%\nostudies\phot\MHP_RADM88	M
Methyl Hydrogen Peroxide Photolysis for JPROC	%M3DATA%\nostudies\phot\MHP_NASA94	M
Organic Nitrate Photolysis for JPROC	%M3DATA%\nostudies\phot\ ORGNIT_RADM88	M
Glyoxal Photolysis to Molecular Hydrogen for JPROC	%M3DATA%\nostudies\phot\ GLYmol_RADM88	M
Acrolein Photolysis for JPROC	%M3DATA%\nostudies\phot\ACROLEIN	M
Cray IEEE MM5 output files used as input to MCIP in the tutorial	%M3DATA%\nostudies\mm5\MET_36\ MMOUT_DOMAIN2	M

APPENDIX D

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Database ObjectStore

ObjectStore Release 5.1 for SPARC Solaris 2.7/SunPro (SunOS 5.4)

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WFTPD

WFTPD (by Texas Imperial Software) 32-bit version 2.40 8/11/1998

Winsock FTP Daemon for MS Windows 3.1, 95 & NT

Operating System - Windows NT

Microsoft, MS-DOS, Windows, Windows NT, ActiveX, BackOffice, and MSN are either

APPENDIX E

CMAQ Model Change Notes

CMAQ Model Change Notes

1. SO2 reactions in CB4 Mechanisms

The CB4 chemical mechanisms originally incorporated in Models-3/CMAQ were based on a version of CB4 used in the UAM-V [Systems Guide to the Urban Airshed Model (UAM-V), Systems Applications International, October, 1993]. That version included a first-order decay reaction of SO2 for simulating sulfate formation via aqueous processes when the latter are not modeled explicitly. As a result, this reaction should not be included in CMAQ versions of the mechanism when CMAQ simulations explicitly include clouds. With this update, all CB4 mechanism configurations in the CMAQ system have been modified such that the rate constant for the reaction <83> (SO2 = SULF) is zero. In addition, the rate constant for reaction <82> (SO2 + OH = SULF + HO2) has been changed from the original UAM-V Arrhenius form to the same Troe form used in the Models-3/CMAQ RADM2 mechanisms and recommended by NASA-JPL (Chemical Kinetics and Photochemical data for Use in Stratospheric Modeling, Evaluation Number 12, National Aeronautics and Space Administration, Jet Propulsion laboratory, California Institute of Technology, January, 1997).

2. Chemical Mechanism Processor Update

The Chemical Mechanism Processor (MP) in Models-3/CMAQ reads a chemical mechanism reactions file (mech.def) and generates two FORTRAN include files (RXDT.EXT and RXCM.EXT) that contain the mechanistic data that are used in CMAQ simulations. Part of those data include rate constant parameters that are sometimes too small to be represented by 32-bit single-precision numbers. As a result, variables holding rate constant parameters were typed REAL*8 to circumvent this problem. In previous releases, these variables were initialized with DATA statements that used E-format. On some compilers (particularly f90 compilers), this procedure will result in some of the small rate constant parameters being initialized to zero rather than their small value. Although effects could vary from compiler-to-compiler, the most probable consequence of this problem is to cause the RADM2 rate constant for the reaction HO2 + HO2 + H2O2 = H2O2 to be too low. To correct this problem, the MP program has been modified to generate rate constant data in D-format for all REAL*8 variables, and all mechanism include files in the archive have been re-generated with the D-format.

3. Aerosol Floating Point Exception Problem

The previous release of the AERO2 module can sometimes result in a floating point exception when the ammonium to sulfate ratio becomes very low. The AERO2 module has been modified to avoid this problem under these conditions.

APPENDIX F

Models-3 Version 4.1 Release Notes
and SMOKE Information

SDC-0002-010-SR-3005
April 3, 2001

RELEASE NOTES OF MODELS-3 (VERSION 4.1)

CONTRACT NO. 68-W-99-002
TASK ORDER NO. 010

Prepared for:

United States Environmental Protection Agency
Office of Research and Development
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CONTENTS

EXHIBITS

1.0 INTRODUCTION

The U.S. Environmental Protection Agency (EPA) is empowered by current legislation to address today's important, grand challenge environmental problems, such as air quality management and linked air and water quality management. The use of environmental models is essential to EPA's cost effective accomplishment of its mission. As part of its High Performance Computing and Communications (HPCC) program, the Agency has initiated the development of a third-generation air quality modeling system called Models-3. Models-3 directly supports the HPCC program goal of using emerging computing and communications technology to:

- Develop the Agency's capability to perform complex multi-pollutant and cross-media pollutant studies that are currently not feasible due to computational limitations.

- Build federal, state, and industrial capabilities to use advanced assessment tools directly responsive to the needs for environmental management.

- Position the Agency to more easily integrate emerging computing and communications technology into environmental assessment tools, ensuring the most reliable and timely response to key environmental issues.

The Models-3 project is one of several being developed under the HPCC program. In many respects, however, Models-3 is the primary focus of EPA's HPCC research activities in that all the other projects under HPCC are, in one way or another, going to make significant contributions to enhance the capabilities of the Models-3 system. The other projects include: 1) linkage of air and water quality models, 2) development and performance evaluation of numerical algorithms on parallel architectures for key environmental processes, 3) development of training and technology transfer approaches to provide state, federal, and industrial air quality scientists and decision makers with credible and useful air quality modeling and decision support tools, 4) implementation of advanced computing hardware, software, and network infrastructure to support HPCC research activities, 5) development of advanced collaboratory visualization and analysis techniques, and 6) outreach activities designed to introduce more EPA researchers to the benefits of HPCC technology in their own areas of interest.

Legal Authority: The High Performance Computing Act of 1991 authorized EPA to perform research directed toward incorporating advances in computing and communications technology into EPA's environmental assessment applications and transferring these advanced tools to key state, federal, and industrial users with decision-making responsibility.

Regulatory Authority: As mandated by Congress in the 1990 Clean Air Act Amendments, the states are required to use photochemical grid models, such as the Urban Airshed Model (UAM) and the Regional Oxidant Model (ROM), to develop credible modeling demonstrations for attaining the National Ambient Air Quality Standards (NAAQS) as part of their State

Implementation Plans.

Regional Acid Deposition Model (RADM) applications are required to support EPA client and policy offices, EPA regional offices, and the states in implementing mandates of the 1990 Clean Air Act Amendments, special agreements between states, and treaty obligations under the U.S.–Canada Air Quality Agreement and the U.N. Economic Commission for Europe. The capabilities of RADM and ROM are improved and incorporated into the Community Multi-Scale Air Quality (CMAQ) model that is a part of the Models-3 Air Quality Modeling framework. CMAQ is a multi-pollutant model, enabling a unified "one-atmosphere" modeling approach and more realistic modeling of chemical interactions in meeting many of the air quality modeling needs of the 1990 Clean Air Act.

1.1 Purpose

This document provides new information not appearing in other Models-3 documentation and discusses changes since the last software release (Version 4.0). Anyone encountering a problem with Models-3 should check this document.

1.2 Scope

This document covers the Models-3 framework, the SMOKE Tool, and problems that may occur in getting to the individual models or tools used in the system. Problems with the actual models or tools are not covered in this document.

1.3 Identification

The sponsor of Models-3 is the National Exposure Research Laboratory (NERL) in EPA's Office of Research and Development. Work on Version 4.1 of Models-3 was performed under Mission Oriented Systems Engineering Support (MOSES) Task Order 002-010. The System Development Center (SDC) product control number for this release is SDC-0002-010-SR-3005.

2.0 REFERENCES

Byun, D.W. and J.K.S. Ching. *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System*. EPA EPA/600/R-99/030, National Exposure Research Laboratory, Research Triangle Park, NC, 768 pp. (1999).

Novak, J.H., R.L. Dennis, D.W. Byun, J.E. Pleim, K.J. Galluppi, C.J. Coats, S. Chall, & M.A. Vouk. *EPA Third Generation Air Quality Modeling System, Models-3 Volume 1: Concept*. EPA/600/R95/084, National Exposure Research Laboratory, Research Triangle Park, NC, 55 pp. (1995).

System Installation and Operation Manual for the EPA Third-Generation Air Quality Modeling System (Models-3 Version 4.1 for Sun Unix and NT), National Exposure Laboratory Research Laboratory, Research Triangle Park, NC, (2001).

EPA Third Generation Air Quality Modeling System, Models-3 Volume 9b: User Manual. EPA/600/R-98/069(b), National Exposure Research Laboratory, Research Triangle Park, NC, 833 pp. (1998) (To Be Updated).

EPA Third Generation Air Quality Modeling System, Models-3 Volume 9c: User Manual: Standard Tutorial. EPA/600/R-98/069(c), National Exposure Research Laboratory, Research Triangle Park, NC, 387 pp. (1998) (To Be Updated).

Revised Project Plan for Implementation Support, Maintenance, and Enhancement of the Third Generation Air Quality Modeling System (Models-3), SDC-0002-010-SR-3001A, September 22, 2000.

3.0 SUMMARY OF FUNCTIONALITY

Models-3 is not a single model or modeling system, but rather a problem-solving environment comprising components that help you build, evaluate, and apply air quality models. Each shaded rectangle shown on Exhibit 1 represents a component that helps you perform major functions associated with environmental modeling.

Models-3's Object Oriented Data Base Management System (OO DBMS) provides a centralized method for managing and sharing data, metadata (information about data), program and/or script executables, and relationships and dependencies among executables and data needed for a specific modeling study. Each of the components communicates with the OO DBMS as shown in Exhibit 1. These components serve as user-friendly tools for accessing or modifying datasets and program source code, developing program or script executables, performing model simulations, and visualizing and analyzing model simulation results.

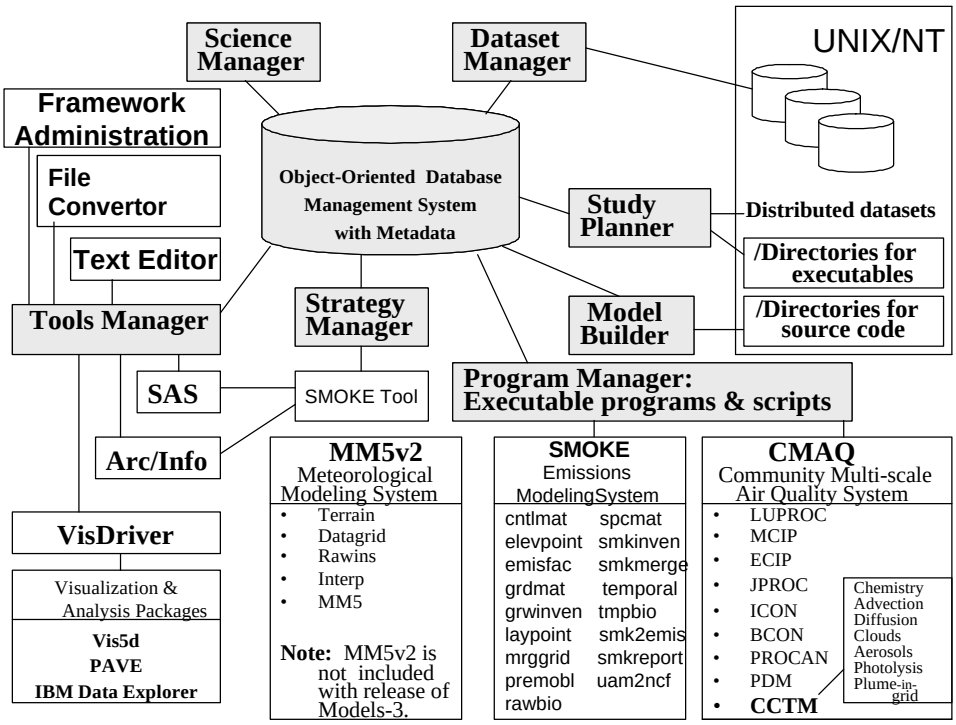

Exhibit 1. Models-3 Framework Components & Integrated Programs

The major Models-3 framework components are:

- **Science Manager** - allows you to define globally shared information on key science components.

- **Dataset Manager** - provides you with the capability to register datasets for use with modeling and analysis programs within Models-3.

- **Study Planner** - allows you to define a study and control the execution of its associated models and processors.

- **Model Builder** - allows you to prepare a model for a specific area for execution. You have the ability to select horizontal grid resolution, vertical layering resolution, and chemical mechanism, without the need for reprogramming.

- **Program Manager** - allows you to register, update, and search for executable programs and/or scripts to make them available for use in defining studies within the Study Planner

component.

- **Strategy Manager** - allows you to interactively execute the SMOKE Tool. SMOKE Tool documentation is available via the Help icon at the Strategy Manager screen.

- **Tools Manager** - accesses a variety of administration, visualization, statistical analysis, and file conversion tools. The tools are Framework Administration (for the Models-3 Administrator), File Convertor, Text Editor, VisDriver (which provides access to Vis5d, Package for Analysis and Visualization of Environmental Data [PAVE], and DXDriver [driver for IBM Data Explorer]), ArcInfo, and Statistical Analysis System (SAS).

4.0 DEGREE OF FUNCTIONALITY PROVIDED

This section provides a list of software changes since the last release, any assumptions or limitations of the Models-3 framework broken down by Models-3 component, and any problems found during testing of the released version.

4.1 Changes Since Last Release

A significant change in this release from the last release is the replacement of the Models-3 Emission Processing and Projection System (MEPPS) model and the Models-3 Emissions Projection (MEPRO) model with the Sparse Matrix Operator Kernel Emission (SMOKE), and the addition of an input processor for SMOKE called SMOKE Tool. The Inventory Data Analyzer (IDA) was deleted in this release as the needed functionality is now included in SMOKE Tool. Changes are included in various Models-3 framework components to accommodate SMOKE and SMOKE Tool; these changes are described in Section 2.0 of Appendix A (SMOKE Tool Documentation). Other changes were also made to correct operational problems, and they are described in the following sections.

4.1.1 Data Base

SMOKE and SMOKE Tool programs were registered into the data base, a SMOKE tutorial study (smkplans_tut36) was added to the data base, and a set of data files (including revised inventories) were included in the release to run the smkplans_tut36 study. The revised inventory files are:

- area/arinv.tut36.ida.txt Area source inventory file
- point/pt.inv.tut36.txt Point source inventory file
- point/psplit.tut36.txt Stack split stack file
- point/pgroup.tut.36.txt Stack split stack group file

4.1.2 Presenter

Numerous updates were made to make the graphical interface more robust.

4.1.3 Study Planner

Changes were made to accommodate the addition of the SMOKE model. See Appendix A.

4.1.4 Science Manager

No changes for this release.

4.1.5 Model Builder

A new version of CHEMMECH is included in this release replacing the previous version. The new version adds a new variable, MECHNAME, as a parameter declaration to the mechanism COMMON include file – RXCM.EXT.

4.1.6 Tools Manager

The File Convertor tool has been revamped. The processor that does Input/Output Application Programming Interface (I/O API) to I/O API, I/O API to ASCII, and ASCII to I/O API conversions was rewritten. It is far more efficient than the previous processor. Conversions from I/O API to SAS format and SAS to I/O API must be done as a two-step process by the user – I/O API to ASCII then ASCII to SAS, or if going the other direction, SAS to ASCII then ASCII to I/O API. The important thing to remember when going from ASCII to I/O API is that the user must click the *Selection* button, then enter information required by the I/O API file header (i.e., Start Date and Time, End Date and Time, Number of Layers, Number of Rows, and Number of Columns).

4.1.7 SMOKE, SMOKE Tool, MEPPS, MEPRO and IDA

MEPPS was removed and replaced by SMOKE. IDA was also removed as the functions needed for SMOKE are incorporated in the added SMOKE Tool. The MEPRO model was removed as SMOKE includes an emissions projection capability.

Information on the installation and use of the SMOKE system and its utilities with Models-3 may be found either in the on-line SMOKE Users Guide (M. R. Houyoux, J. M. Vukovich, and J. E. Brandmeyer, 2001), or in the same document in pdf format contained in the tar (compressed) file containing the SMOKE code. These are maintained by the SMOKE developer, MCNC North Carolina Supercomputing Center, on the internet at http://iceis.mcnc.org/.

SMOKE Tool has four basic functions:

- Emission Chemical Mechanism Preparation.
- Emission Inventory Preparation.
- SMOKE Input File Preparation.
- Grid Spatial Surrogate Preparation.

The main SMOKE Tool screen, accessed via the Models-3 Strategy Manager, starts the first three functions. Individual functions within the SMOKE Tool have the ability to register datasets produced with the Models-3 Dataset Manager. SMOKE Tool documentation is included in this document as Appendix A. Grid Spatial Surrogate Preparation is executed in batch mode via one or more study plans registered using the Models-3 Study Planner. Grid Spatial Surrogate Preparation is included in Appendix A. The SMOKE Tool documentation in Appendix A is accessible in Models-3 Version 4.1 by selecting the Help icon at the Strategy Manager main screen.

The land-use gridding program in SMOKE Tool creates an I/O API format file which can be used as input to BEIS3. Some users may be using BEIS2 rather than BEIS3. Therefore, a program, BEIS 3to2, was added to SMOKE Tool to convert the I/O API file to be BEIS2 readable. The user can select the I/O API files from the SMOKE Tool land-use gridding program for input to BEIS3, or the user can select the ASCII files output from the BELD3to2 SMOKE Tool program for input to BEIS2.

4.2 Assumptions, Limitations, and Problems

The following paragraphs present assumptions, limitations, and problems with various Models-3 components.

4.2.1 Presenter

This section addresses common problems found in the graphical interface of the Models-3 framework.

- If you have selected a remote host that has been registered as Orbix-enabled but Orbix is not running, problems can occur, and the Models-3 framework may crash.

- The print function will not work properly in certain complex windows. The problem appears in the Galaxy libraries. No immediate action is planned to remedy the problem.

- Every object (e.g., dataset, program, etc.) has a unique identification (ID) that you normally would not need to know. However, when uniqueness is required, the ID can assist you in distinguishing among different objects with the same name. You can reveal

the IDs in both the summary and detail windows. Simply enlarge the summary windows and an ID column will appear. In the detail windows, go to the menu bar, click *View*, and select *Hidden Info*. An informational pop-up window that includes the ID will appear.

- If you exit while a save is in progress, an "object not saved" type of message appears. You should select *Cancel* and wait to avoid any problems. If the object has been saved, a "saved successfully" type of message is displayed. If you have saved an object but it has taken a while and no message has appeared, the object can be saved again.

- **User Hint:** Save frequently when adding or changing information. As an example, in Study Planner when annotating file links you may have many file links to annotate in a plan. A good rule of thumb is you should not annotate more than three links without doing a Save.

- On rare occasions, the Orbix daemon may get suspended when it is started directly from Unix. This is sometimes caused by Concurrent Versions System (CVS). You should always use the "m3run" script to keep this from happening.

- When an object other than a dataset is copied, the server thinks it is editing the original object. If the original object is edited before the copy is saved, the message "Someone else is editing this object" is displayed. The message can be ignored. After saving the object, the message will not appear again.

- When using the NT or X-Window emulators, the system pauses and waits for you to do something. If the mouse is moved, the system will continue. This is a problem in the Galaxy library and cannot be fixed at this time. **It is important to occasionally move the mouse when long operations are occurring. This situation occurs frequently in the NT version when a node is being executed in Study Planner and it is time to update the screen.** The execution does not stop, but you will not know the current status of the execution until the mouse is moved.

- Find screens will accept more than 16 characters in a Name (Dataset, Study, Plan, Program, etc.) field. Creation screens limit the names to 16 characters. The user should never enter more than 16 characters for a Name on a find screen.

- On the NT, if Models-3 is not acting normally (e.g., you are having trouble doing a Save), there is a possibility that one of the Models-3 subsystems has aborted. Exit Models-3 when this happens. Next focus on the orbix window and do a <**Ctrl C**>. Then exit the two windows that were being used by Models-3, start up two new windows, and reinitiate Models-3.

4.2.2 Dataset Manager

- When selecting *Dataset/Visualize* at the menu bar of a Dataset Detail Window, a Vis5d format file is expected unless the file is in I/O API format. If the file format is I/O API, the VisDriver Program is displayed automatically. To use an I/O API format file, VisDriver from the Tools Manager can also be used.

- The *Dataset/Move* does not catch the error when you specify a file that is really the same file but different hosts were provided. (The file is mounted on both hosts.)

4.2.3 Study Planner

- On rare occasions when executing a plan, a warning message displays stating that "The Study Planner has experienced a problem and has restarted. It will no longer provide you with feedback ...." If this message occurs, you should click on the warning message *OK* button, select the Plan tab, then copy the selected plan (i.e., at menu bar click *Edit* > *Copy* > *Paste*), then select the New plan, click the Details icon, rename the New plan, and Save. Execution from the copy of the original plan should proceed without a problem. You should delete the original plan, and you can rename the New plan back to the original plan name.

- When copying selected nodes, datasets, or both with their connected edges from one plan to another, the edges are not correctly updated visibly on the screen when an individual node or dataset is moved. This is corrected after saving and refreshing the study.

- When clearing an environment variable that is a higher-level environment variable (i.e., a study or plan level) from the Node Properties screen, the environment variable will not be displayed when going back into the Node Properties until some other action is done (e.g., pressing *OK* on the Node pop-up then coming back in).

- You cannot get a file from, or put one to, a non-Orbix-enabled machine that does not have a "models3" user by using a data source or sink when the execution of the connected node is not done on that machine. This is because Models-3 does not have a user ID and password for that machine. A dummy node can be created on the remote machine that allows the file to be specified as the output (or input, if using as a sink).

- You cannot copy a file between two non-Orbix-enabled machines if they do not use the same ID/password.

- Models-3 will abort if the user attempts to 'Exit' a plan when there is still an active Annotate Link Properties screen for the plan. The work-around is to 'Exit' all Annotate Link Properties screens displayed for a plan before exiting the plan detail screen.

- There are five places where the execution host can be set in Models-3 that can affect a plan execution -- in program registration, at a study detail window, at a plan detail window, and when annotating file links (both 'To' and 'From') at the Define Physical File Location screen. In the Execution Host pick list selection, a user can select [Default Host] from the list and the host name is displayed within square brackets. The user can also explicitly select the same host in the list whereby the host is displayed without brackets. **Be consistent in the way you select the host (i.e., default or explicit)**. The reason for this is Models-3 Study Planner sometimes does not recognize that the host name in square brackets assigned in one place is the same as the same host name assigned without the square brackets. Being inconsistent can cause Study Planner to hang in execution, overwrite a file (Unix platform), attempt to write to the wrong drive (NT platform), or cause Models-3 to request the user to enter a password. An additional measure of protection against overwriting files should also be taken by making static input files (e.g., CEM data and inventory files) to **not** have write permission.

- **User Hint**: In Study Planner, when annotating an input file link at the Link Information screen, there is a 'From' link and a 'To' link (below the 'From' link). If using the pick lists to select the files, select the 'To' pick list button before the 'From' pick list button to view the list of input logical file names specified for the program assigned to the node.

- **User Hint:** In Study Planner, when annotating physical file links, use the 'Physical File' pick list button then select 'Filter' at the Select File window. By using the filtering capability to establish a file path and name instead of typing them in, you eliminate the possibility of a typographical error.

4.2.4 Strategy Manager

There are no known problems.

4.2.5 Program Manager

- A physical file is not deleted when delete is selected. By design, only the metadata is deleted.

4.2.6 Science Manager

- If data is entered for the horizontal grid specifications that do not allow the grid to be viewed, an error message is displayed in the Orbix window.

- In the Vertical Layering Detail Window, you can generate the vertical layers as many

times as you want. Once the metadata is saved, you cannot change the vertical layering type or regenerate the vertical layers. However, you can add to or otherwise modify the existing vertical layers.

- When editing two horizontal coordinate systems at the same time, only one projection parameters pop-up window can be displayed at a time.

- When copying a coordinate system at the Coordinate System detail page, after selecting a coordinate system to copy, you must first click on the *Projection* button and then *Component/Copy* at the menu bar. If you do not first click on the *Projection* button, the projection parameters will not be included in the copy.

- For GridViewer to work in the NT version, an X-Window server must be on the system, and the X-Window server must have been already initiated by the user. GridViewer is the program run when *View Grid* is selected on the Grid Definition tabbed page of the Horizontal Grid Manager.

4.2.7 Model Builder

- When you do a Model Build, the system issues a "The model has been generated" message when the build execution completes. The system does not determine, though, if errors were in the build itself. You should click the *View Build Log* and *View Compile Log* buttons after the message is issued to be sure that no errors are in the logs.

- **Note:** Model Builder is not implemented for the Cray computer.

4.2.8 Tools Manager

- In order to bring up VisDriver on NT, both Interix and an X-Window server must be on the system, and the X-Window server must have been already initiated by the user.

4.2.9 Execution Manager

There are no known problems.

4.2.10 File Migrator

- For File Migrator to function best, there should be a "models3" user on all Unix systems. Also, the M3TEMP directory should be a mounted directory if using a machine other than the one the servers are on.

- Remember that to function properly on Unix systems, the .rhosts file of each user of any

non-Orbix-enabled machine must allow access to both the user and the machine that is running the File Migrator. Please refer to the *System Installation and Operation Manual for the EPA Third-Generation Air Quality Modeling System (Models-3 Version 4.1 for Sun Unix and NT)* for more instructions.

4.2.11 Help

- Help is displayed through an Internet browser. Your system must have a default browser installed to see Help. Also, the browser must take a command line argument. If the browser is already started, the system will not "un-iconize" it and bring it to the front.

- *Index* and *Tutorial* from the Help pull-down menu are not implemented.

4.2.12 File Convertor

- When using free format and specifying a Fw.d format, the w (width) is ignored, and the display for a value less than 1 is 0.xx with d decimal accuracy.

- Free format using a blank delimiter has been changed to process multiple blanks as one delimiter.

- **Note:** File Convertor has the ability to do simple units conversions where the conversions are a multiplicative factor. By design it does not have the ability to do conversions where more than just a multiplicative factor is involved [e.g., C = 5/9 (F - 32)]. Therefore, in File Convertor at the Describe Variable screen, you will not find 'Temperature' in the Category pick list. File Convertor does not have the ability to convert between different temperature scales.

- The process of converting between SAS format and I/O API format files described in the Models-3 user manual no longer applies. The way to convert between SAS and I/O API files is a two step process. Do one run converting from I/O API (or SAS) to ASCII, and then do a second run converting from ASCII to SAS (or I/O API).

- I/O API files have a header containing temporal, gridding, and vertical layering information. To do an ASCII to I/O API or I/O API to I/O API file conversion, this information is entered via the Select Criteria screen accessed by clicking the *Selection* button at the File Convertor main screen.

5.0 INSTALLATION INSTRUCTIONS

Please refer to *System Installation and Operation Manual for the EPA Third-Generation Air Quality Modeling System (Models-3 Version 4.1 for a PC NT Operating System).*

APPENDIX F-1

SMOKE TOOL DOCUMENTATION

CONTENTS

1. SMOKE TOOL

The SMOKE Tool is an input processor for SMOKE, executed in part via Strategy Manager. The tool has four basic functions:

- Emission Chemical Mechanism Preparation.
- Emission Inventory Preparation.
- SMOKE Input File Preparation.
- Grid Spatial Surrogate Preparation.

2. Grid Spatial Surrogate Preparation

The primary purpose of the grid processor is to generate spatial surrogates for SMOKE horizontal gridding. The grid processor is executed through nodes in a study plan. The underlying functions that the grid processor executes are modified versions of the Statistical Analysis System (SAS) and ArcInfo gridding programs copied from the MEPPS Emission Processor (EMPRO). The grid processor performs the following functions:

- Define Grid — Creates the grid workspace, receiving the grid description file from the Study Planner. The program creates the grid directories, imports the grid description, and generates the base Geographic Information System (GIS) coverages in the workspace. The grid description is read from file G_GRIDPATH (supplied from the study planner).

- Generate Coverages — Generates GIS coverages in the workspace. The user selects the coverages to generate through environment variables. The names of the environment variables are based upon the GIS coverages defined to the SMOKE Tool.

- Generate Surrogates — Computes spatial surrogates for the grid from the GIS coverages generated for the grid. The user selects the coverages to include in the surrogate calculation through environment variables. The program computes all spatial surrogates defined for each coverage selected.

The grid processor creates the grid directories in a user-specified location. The location is specified through the following environment variables:

- EMS_HOME — Workspace Path. The base directory under which the grid information is stored. Supplied by user.

- HGRIDNAME — Models-3 Grid Name. The grid name is used to define subdirectories under the workspace path for the grid. Supplied by

Study Planner.

All data for the grid, created by the Define Grid and Generate Coverages functions, is stored in subdirectories under directory **$EMS_HOME/gridspec/$HGRIDNAME**. The user specifies the location of the spatial surrogate file, created by the Generate Surrogate function, in a plan output file specification.

The user defines the GIS coverages available to SMOKETOOL through the following environment variables:

- GISDB — Name of the GIS data base directory. This directory contains the GIS coverages and related data files for the surrogate processing.
- COVER_DEF — Name of the file containing the coverage definition table. This table defines the GIS coverages available for surrogate processing.

The initial GIS coverages released with Models-3 are:

• COUNTY	County areas	
• CENSUS	Census tract/block group areas	(US only)
• FHAROAD	FHA road lengths	(US only)
• AGRICULTURE	Agricultural areas	(US only)
• AIRPORTS	Airport locations	
• PORTS	Port locations	
• RAILROADS	Railroad lines	
• LAND_WATER	Land-water areas	
• URBAN-RURAL	Urban-rural areas	
• ROADS	Road lengths	
• FOREST	Forest areas	
• TIGER	TIGER/Line roads	(US only)

To select a coverage, set the environment variable for the coverage to YES or Y. The value may contain upper or lower case letters. Sample environment variable settings that cause coverages to be processed are:

```
PORTS=Y
AIRPORTS=YES
RAILROADS=yes
```

The surrogates step also uses the following environment variables:

- FEATURE_SRG Name of the Feature-Surrogate Table. This table defines the manner in which spatial surrogates are computed from the coverage features.

- CENSUS_DATA Name of the Census Data File. This file contains housing and population data associated with the CENSUS coverage. It may also contain state or county level data.

- FEAT_STCY_FRAC Name of the Census State-County Fraction table. This file contains fractions to allocate state level census data to the counties within the states.

- SURROGATES Name of the spatial surrogates file. This contains the spatial surrogates (or gridding coefficients) computed in the surrogates step.

The follow sections describe the various directories, GIS coverages, and files used in the spatial surrogate processor.

3. Grid Directories

The grid master directory is **$EMS_HOME/gridspec/$EMS_GRID**. The subdirectories created are shown in the following table:

Subdirectory	Type of Data	Environment Variable	SAS Reference
common/sas	Ungridded Emissions	EMS EMS_CVRT	library EMS file EMS_CVRT
common/gis	Ungridded GIS	EMSG	file EMSG
sas	Gridded Emissions	EMS_GRD EMSF_GRD	library EMS_GRD file EMSF_GRD
gis	Gridded GIS	EMSG_GRD	file EMSG_GRD

The first two directories contain data for the grid's geographic area that have not been processed for a grid. The EMSG directory contains GIS coverages that have not been overlaid with a grid.

The gridded data directories contain data that have been processed for the grid. EMS_GRD contains the grid description and gridded data files. The EMSG_GRD directory contains GIS coverages that have been overlaid with the grid.

4. SMOKE Input File Generation

The SMOKE Tool generates the following input files for SMOKE:

- Temporal Profiles.
- Temporal Cross-References.
- Gridding Cross-References.
- Area and Point Source Control Files.
- Speciation Cross-References.
- Pollutant File (SIPOLS).
- MOBILE Emission Factor Cross-Reference (MPLIST).

SAS is used to generate the input files for SMOKE. The individual files contain a number of packets. Each packet contains a set of different fixed-format records. SAS routines are used for data checking, sorting, and merging the packet data into the full files.

Some additional files that are not handled in the tool are the ACTRACK, PCTRACK, and MPREF files. The ACTRACK and PCTRACK files identify sources to include in the control reports. These are simple, free-form ASCII files that list the counties and Source Classification Codes (SCC) for the report. Screens could have been generated to input these lists, but it is simpler for the user to type the lists directly and annotate the report node with the file name. The MPREF file defines the MOBILE5 inputs for SMOKE. It contains the statements that define SMOKE emission factor sets and imbedded MOBILE5 input statements.

The following sections describe the files processed in the SMOKE input processor of the SMOKE Tool. In most cases the tool allows the users to load pre-existing data, modify the data, check the packet data for data value errors, and cross-check the data in different packets.

5. Study Planner

Changes were made to the Study Planner to get the necessary information to SMOKE. The information that SMOKE must get at the time of the execution of the program is:

- Grid Information (including horizontal grid, coordinate, and vertical layer information).
- Case Information.
- Chemical Mechanism Information.
- Extracted Continuous Emission Monitoring (CEM) Data for Case.
- File Lists for SMOKE Input.

6. Grid Information

In the past, Study Planner did not allow selection of grid information because Model Builder compiled the grid information directly into the FORTRAN code. This caused the program to require compiling every time the grid was changed. To implement SMOKE and other programs so that the executables do not require recompiling every time, the grid information from the Science Manager was made available to the SMOKE program.

7. Case Information

Currently, Study Planner sends the case information in environment variables. There are four environment variables as follows:

- G_STDATE Julian Date in YYYYDDD format.
- G_STTIME Time in HHMMSS format.
- G_TSTEP Time step in HHMMSS format.
- G_RUNLEN Run length in HHMMSS format.

YYYY is the four-digit year. DDD is the number of days since the beginning of the year. HH is the hours (this does not have to be two digits; it can be any number of digits). MM is the minutes (two digits). SS is the seconds (two digits).

8. Chemical Mechanism Information

Chemical mechanism information is passed to SMOKE as it is executed in Study Planner. This is done using the same idea discussed in Section 2.1, Grid Information. The files are created, and environment variables provide the location of these files. In addition, CHEMMECH outputs the RXCM.EXT and RXDT.EXT files into one file in the same format as was discussed in Section 2.1. The environment variable name is C_RX for the file created by CHEMMECH and C_TABLE for the remaining chemical mechanism files. The chemical mechanism is a selection at the study and plan levels.

9. Extracting CEM Data for Case

A specific SAS program was developed and is executed as a node in a plan. The program has two inputs:

- The Models-3 case description annotated to the node via environment variables G_STDATE, G_STTIME, and G_RUNLEN.

- A CEM dataset (SAS) specified through an input link. The user has to annotate the link, selecting a registered CEM dataset that contains data for the case period.